Open Systems

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A general feature of electron devices is that they are of use only when connected to a circuit, and to be so connected any device must possess at least two terminals, contacts, or leads. As a consequence, every device is an open system with respect to carrier flow [1]. This is the overriding fact that determines which theoretical models and techniques may be appropriately applied to the study of quantum devices. For example, the quantum mechanics of pure, normalizable states, such as those employed in atomic physics, does not contribute significantly to an understanding of devices, because such states describe closed systems.

To understand devices, one must consider the un-normalizable scattering states, and/or describe the state of the device in terms of statistically mixed states, which casts the problem in terms of quantum kinetic theory. As a practical matter of fact, a device is of use only when its state is driven far from thermodynamic equilibrium by the action of the external circuit. The non-equilibrium state is characterized by the conduction of significant current through the device and/or the appearance of a non-negligible voltage drop across the device.

In classical transport theory, the openness of the device is addressed by the definition of appropriate boundary conditions for the differential (or integro-differential) transport equations. Such boundary conditions are formulated so as to approximate the behavior of the physical contacts to the device, typically Ohmic or Schottky contacts [2]. In the traditional treatments of quantum transport theories, the role of boundary conditions is often taken for granted, as the models are constructed upon an unbounded spatial domain. The proper formulation and interpretation of the boundary conditions remains an issue, however, and will be examined in the present work. It should be understood that, unless otherwise specified, all models to be considered here are based upon a single-band, effective-mass Schrodinger equation.

1. Tunneling Theory

The simplest model of quantum transport in devices is to describe the problem in terms of the scattering of the electron wavefunction by a spatially varying potential. One assumes that this potential is situated between two electron reservoirs, each of which emits particles with an equilibrium distribution into the scattering region. The reservoirs will, in general, have different chemical potentials, their difference representing an applied bias voltage. The net flux of electrons passing between the reservoirs

constitutes the electrical current conducted by the device. A single-particle Schrodinger equation can only describe a situation in which the electrons move perfectly coherently throughout the device. Any loss of coherence due to inelastic collisions requires a higher-level description. Nevertheless, the solutions of Schrodinger's equation remain one of the fundamental tools available to understand and predict the behavior of quantum-scale devices.

In this section we will first show that all particles with $E<V_0$ incident on a potential step of height V_0 are reflected. In other words, although the quantum-mechanical treatment predicts penetration of the wavefunction into the classically-forbidden region (the probability density in this region is non-zero), we can not demonstrate this phenomenon in a laboratory. However, one can demonstrate the penetration into a classical-forbidden region if we chop-off the potential step, changing it into a barrier of width L. Then, according to quantum physics, particles with $E<V_0$ incident on the barrier from the left, will penetrate the potential and will be transmitted into the classically-allowed region where we can detect them. This wholly non-classical phenomenon is called TUNNELING (see Figure 1-16) []. The two remarkable applications of tunneling are:

(a)   Resonant tunneling diodes, which are used as switching units in fast electronic circuits.

(b)   Scanning tunneling microscope (STM), based on the penetration of electrons near the surface of a solid sample through the barrier at the surface (see Figure 1-17). These electrons form a "cloud" of probability outside the sample. Although the probability of detecting one of these electrons decays exponentially with distance (from the surface), one can induce and measure a current of these electrons and attain a magnification factor of 100 million - large enough to permit resolution of a few hundredths the size of an atom. Gerd Binning and Heinrich Rohrer won the Noble Prize in Physics in 1986 for the invention of the STM [3].
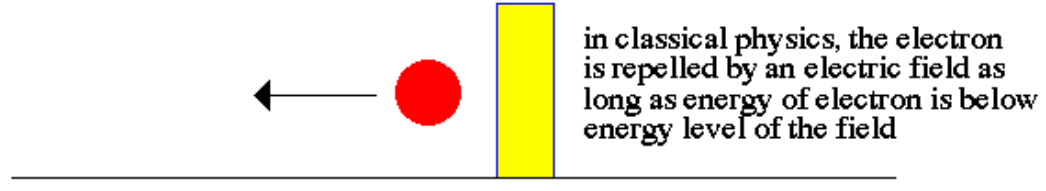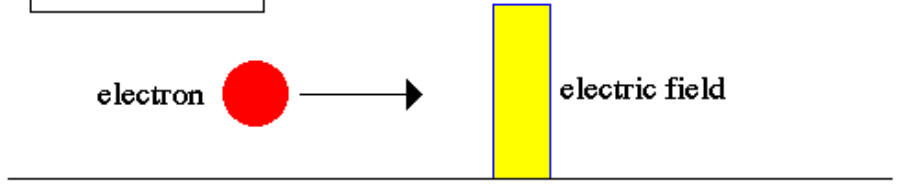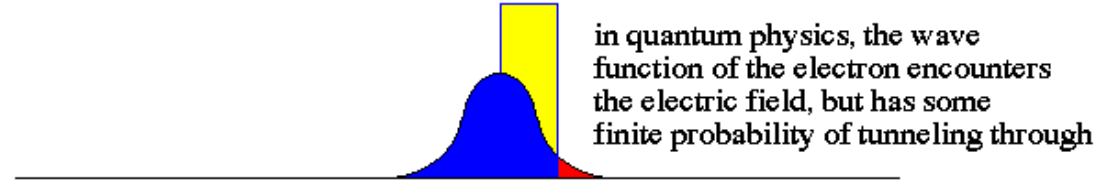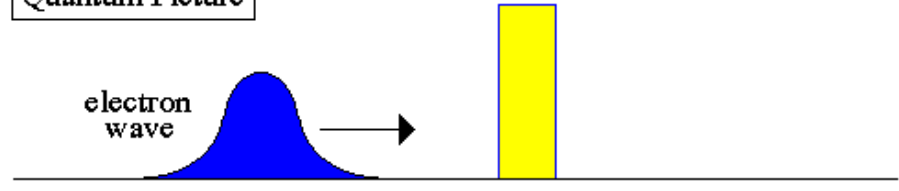
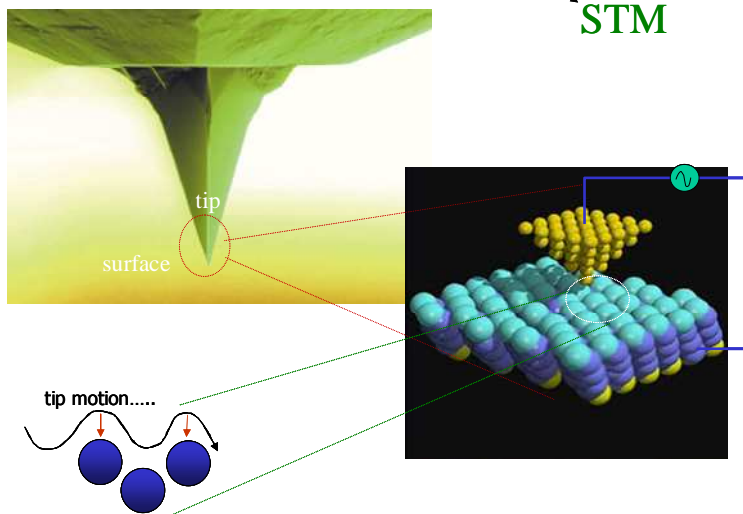Figure 1. Quantum-mechanical tunneling.

Figure 2. Scanning tunneling microscope operation based on quantum-mechanical tunneling.

In the rest of this section, we will first describe the tunneling phenomenon through the example of a single barrier. Then, we will talk about multiple barrier case formulation, the double barrier being a special case which we have in resonant tunneling diodes.

2.   General Notation

Quantum physicists are interested in all kinds of physical systems (photons, conduction electrons in metals and semiconductors, atoms, etc.). States of these rather diverse systems are represented by the same type of functions, the state functions [4]. The *first postulate of quantum mechanics* states that *every physically-realizable state of the system is described in quantum mechanics by a state function ψ that contains all accessible physical information about the system in that state.* Physically realizable states are states that can be studied in laboratory, accessible information is the information we can extract from the wavefunction, and the state function is function of position, momentum and energy that is spatially localized. *Also*, if ψ_1 and ψ_2 represent two physically-realizable states of the system, then the linear combination

$$\psi = c_1\psi_1 + c_2\psi_2 , \qquad\qquad (1)$$

where c_1 and c_2 are arbitrary complex constants, represents a third physically realizable state of the system.

Quantum mechanics describes the outcome of an ensemble of measurements, where an ensemble of measurements consists of a very large number of identical experiments performed on identical non-interacting systems, all of which have been identically prepared so as to be in the same state. This brings

us to the **second postulate of quantum mechanics** that states: *If a system is in a quantum state represented by a wavefunction ψ, then*

$$PdV = |\psi|^2 \, dV \qquad\qquad (2)$$

is the probability that in a position measurement at time t the particle will be detected in the infinitesimal volume dV. Note that $|\psi(x,t)|^2$ is the position and time probability density. The importance of normalization follows from the Born interpretation of the state function as a position probability amplitude. According to the second postulate of quantum mechanics, the integrated probability density can be interpreted as a probability that in a position measurement at time t, we will find the particle anywhere in space. Therefore, the normalization condition for the wavefunction is:

$$\int PdV = \int |\psi(x, y, z)|^2 \, dV = \int \psi^*(x, y, z)\psi(x, y, z)dV = 1 \qquad\qquad (3)$$

There are several limitations on the wavefunction that arise from this normalization condition: (1) Only normalizable functions can represent a quantum state and these are called physically admissible functions. (2) State function must be continuous and single valued function. (3) State function must be a smoothly-varying function (continuous derivative).

The Born interpretation of quantum mechanics enables us to determine from a wavefunction, the probabilistic information. For example, we can answer the following question: In an ensemble measurement of position at time t, what is the probability that a member of the ensemble will exhibit a value in the range from x to $x+dx$? To characterize the results of an experiment, we use two statistical quantities: ensemble average $<x>$ and standard deviation Δx. In quantum theory, the ensemble average of an observable for a particular state of the system is called the expectation value of that observable that is calculated using

$$<x> = \int xP(x,t)dx = \int \psi^*(x,t)x\psi(x,t)dx = (\psi, x\psi) \qquad\qquad (4)$$

Note that the expectation value can be time dependent, i.e. $<x>=<x(t)>$. Also, the expectation value depends upon the state of the system. Different states, represented by different state functions have different ensemble averages. Let's denote a generic observable Q(x) that depends only upon position. The expectation value of this observable is given by:

$$<Q(t)> = \int \psi^*(x,t)Q(x)\psi(x,t)dx \qquad\qquad (5)$$

The other statistical quantity that one uses in quantum physics is the standard deviation of an observable - otherwise known as uncertainty. For a position measurement, the uncertainty in x answers the following question: In an ensemble measurement at time t of the position of a particle in a state $\psi(x,t)$, what is the

spread of the individual results around the expectation value <x>? To answer this question, one needs to calculate the dispersion:

$$\Delta x^2 = \int \psi^*(x,t)[x-<x>]^2 \psi(x,t)dx = <x^2> - <x>^2 \qquad (6)$$

The uncertainty, or the standard deviation is given by:

$$\Delta x = \sqrt{<x^2> - <x>^2} \;, \qquad (7)$$

or the uncertainty equals the square-root of the dispersion. In general, the uncertainty in the measurement of the observable $Q(x)$ is given by:

$$\Delta Q = \sqrt{<Q^2> - <Q>^2} \qquad (8)$$

We have already stated that $\psi(x,t)$ is the state function of a system in the position representation. It must be normalizable since it describes a localized particle. Therefore, one can define a Fourier transform of this function:

$$\psi(x,0) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} dk e^{ikx} \phi(k), \qquad (9)$$

where $\phi(k)$ is the Fourier coefficient, or in this particular case it represents the momentum wavefunction also known as the amplitude function. The description of the particle in momentum state is achieved using these momentum wavefunctions. In summary, the position probability amplitude $\psi(x,t)$ and the momentum state function $\phi(k)$ are state descriptors for a microscopic system. The second class of basic elements are the observables, which represent the physical attributes of a system that can be measured in a laboratory. Examples of observables are position $x(t)$, momentum $p(t)$ and energy $E(x(t))$. The problem of applying a classical definition of observables for quantum states is that it is impossible to measure the properties of a microscopic system without altering its state. ***The third postulate of quantum mechanics*** states that: *Every observable in quantum mechanics is represented by an operator which is used to obtain physical information about the observable from the state function*. For an observable that is represented in classical physics by a function $Q(x,p)$, the corresponding operator is $Q(\hat{x}, \hat{p})$ [5].

Table 1. Most important operators in quantum Physics.

Observable	Operator
Position	$\hat{x}$
Momentum	$\hat{p} = \dfrac{\hbar}{i}\dfrac{\partial}{\partial x}$
Energy	$E = \dfrac{\hat{p}^2}{2m} + V(\hat{x}) = -\dfrac{\hbar^2}{2m}\dfrac{\partial^2}{\partial x^2} + V(x)$

An operator (see Table 1-4) is an instruction, a symbol which tells us to perform one or more mathematical acts on a function, say $f(x)$. The essential point is that they act on a function. Operators act on everything to the right, unless the action is constrained by brackets. The addition and subtraction rule for operators reads:

$$\left(\hat{Q}_1 \pm \hat{Q}_2\right)f(x) = \hat{Q}_1 f(x) \pm \hat{Q}_2 f(x) \qquad (10)$$

The product of two operators implies successive operation:

$$\hat{Q}_1 \hat{Q}_2 f(x) = \hat{Q}_1\left[\hat{Q}_2 f(x)\right] \qquad (11)$$

The product of two operators is a third operator:

$$\hat{Q}_3 = \hat{Q}_1 \hat{Q}_2 \qquad (12)$$

Two operators commute if they obey the simple operator expression:

$$\left[\hat{Q}_1, \hat{Q}_2\right] = \hat{Q}_1 \hat{Q}_2 - \hat{Q}_2 \hat{Q}_1 = 0 \;\;\Rightarrow\;\; \hat{Q}_1 \hat{Q}_2 = \hat{Q}_2 \hat{Q}_1 \qquad (13)$$

The requirement for two operators to be commuting operators is a very important one in quantum mechanics and it means that we can simultaneously measure the observables represented with these two operators. The non-commutivity of the position and the momentum operators (the inability to simultaneously determine particles position and its momentum) is represented with the Heisenberg uncertainty principle, which in mathematical form is expressed as:

$$\Delta x \cdot \Delta p \geq \frac{\hbar}{2} = \frac{1}{2}\left|\left\langle\left[\hat{x}, \hat{p}\right]\right\rangle\right|, \qquad (14)$$

and can be generalized for any pair of observables.

In 1926 Erwin Schrödinger [6] proposed an equation that describes the evolution of a quantum-mechanical system (which represents quantum equations of motion), and is of the form:

$$-\frac{\hbar^2}{2m}\frac{\partial^2\psi}{\partial x^2}+V(x)\psi(x,t)=\left[-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}+V(x)\right]\psi(x,t)=i\hbar\frac{\partial\psi}{\partial t} \qquad (15)$$

This work of Schrödinger was stimulated by a 1925 paper by Einstein on the quantum theory of ideal gas [7], and the de Broglie theory of matter waves [8]. Examining the time-dependent SWE, one can also define the following operator for the total energy:

$$\widehat{E}=i\hbar\frac{\partial}{\partial t} \qquad (16)$$

The introduction of the Schrodinger equation brings us to the ***fourth fundamental postulate of quantum mechanics*** which states that *the time development of the state functions of an isolated quantum system is governed by the time-dependent SWE* $\widehat{H}\psi=i\hbar\partial\psi/\partial t$, *where* $\widehat{H}=\widehat{T}+\widehat{V}$ *is the Hamiltonian of the system*. The time-dependent Schrödinger wave equation (TDSWE) describes the evolution of a state provided that no observations are made. An observation alters the state of the observed system, and as it is, the TDSWE can not describe such changes.

The solution of the TDSE is a rather formidable problem even in 1D. The underlying problem is not just that it is a partial differential equation of second order in *x* and first order in *t*, but that we must consider both of these variables at once. As a consequence, the space and time dependence of the wavefunction may be very complicated. One way to solve the TDSE is to seek solutions that have a particularly simple form, i.e.

$$\psi(x,t)=\psi(x)\xi(t) \qquad (17)$$

These product functions are called separable solutions of the partial differential equation (PDE). In Quantum Mechanics, they are called stationary-state wavefunctions [9]. One can find these stationary-state wavefunctions using a method called separation of variables. For example, substituting the above expression for $\psi(x,t)$ into the TDSE, one gets:

$$\xi(t)\left[-\frac{\hbar^2}{2m}\frac{\partial^2\psi(x)}{\partial x^2}+V(x,t)\psi(x)\right]=\psi(x)i\hbar\frac{\partial\xi(t)}{\partial t} \qquad (18)$$

or:

$$\frac{1}{\psi(x)}\left[-\frac{\hbar^2}{2m}\frac{\partial^2\psi(x)}{\partial x^2}+V(x,t)\psi(x)\right]=i\hbar\frac{1}{\xi(t)}\frac{\partial\xi(t)}{\partial t} \tag{19}$$

The last equation is almost separable, since, in general, the potential energy can depend on both x and t. If we assume that $V(x,t)=V(x)$, i.e. the potential energy is time-independent, then the LHS is only a function of x and the RHS is only a function of t. Therefore, the two sides can be equal if they are constant. This gives us two equations:

$$\begin{cases}\dfrac{1}{\psi(x)}\left[-\dfrac{\hbar^2}{2m}\dfrac{\partial^2\psi(x)}{\partial x^2}+V(x)\psi(x)\right]=\alpha\to-\dfrac{\hbar^2}{2m}\dfrac{\partial^2\psi(x)}{\partial x^2}+V(x)\psi(x)=\alpha\psi(x)\\[2mm]i\hbar\dfrac{1}{\xi(t)}\dfrac{\partial\xi(t)}{\partial t}=\alpha\to i\hbar\dfrac{\partial\xi(t)}{\partial t}=\alpha\xi(t)\end{cases} \tag{20}$$

The fact that we can obtain these two equations at all, provided that V does not depend on time, proves that stationary state wavefunctions exist for systems with a time-independent potential energy. A system whose potential energy is time-independent is said to be conservative. Hence, stationary states exist for conservative systems.

Now, the solution of the second equation [for $\xi(t)$] is very simple, and is given by:

$$\xi(t)=\xi(0)e^{-i\alpha t/\hbar} \tag{21}$$

The Born interpretation of $\psi(x,t)$ [10] provides a clue to the physical meaning of the separation constant α. The wavefunction of a stationary state oscillates at a frequency $\omega=\alpha/\hbar$. From the de Broglie-Einstein relation, one has that $E=\hbar\omega=\alpha$. Hence, we can represent α as the total energy of the particle in the state represented with this wavefunction, i.e.

$$\xi(t)=\xi(0)e^{-iEt/\hbar} \tag{22}$$

The first equation then becomes:

$$\left[-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}+V(x)\right]\psi_E(x)=E\psi_E(x) \tag{23}$$

This is the time-independent SE (TISE), which is an equation of a very special form. There is a differential operator representing the total energy of the system, which operates on the unknown function $\psi_E(x)$ to produce the same function $\psi_E(x)$ multiplied by a parameter E. Mathematicians call an equation of this form an eigenvalue equation where $\psi_E(x)$ is the eigenfunction and E is the corresponding eigenvalue.

Thus, the results presented in this section can be summarized as follows: (1) If a microscopic system is conservative, then there exist special quantum states of the system, called stationary states, in which the energy is sharp. (2) Even if the number of these eigenstates is infinite, the energies of the bound states form a discrete list. (3) If there is a one-to-one correspondence between the quantized energies of a quantum system and its bound state, or stationary-state wavefunctions, then the bound state energy is non-degenerate.   If there are stationary states for which there correspond more than one distinct spatial functions, such bound states are called degenerate.

2.1   Stationary States for a Free Particle

Let's try to solve the TISE for a free particle, for which $V(x) = 0$, i.e.

$$-\frac{\hbar^2}{2m}\frac{\partial^2 \psi(x)}{\partial x^2} = E\psi(x) \rightarrow \frac{\hbar^2}{2m}\frac{\partial^2 \psi(x)}{\partial x^2} + E\psi(x) = 0 \qquad (24)$$

This is a homogeneous, second-order partial differential equation with constant coefficients, and the solution of this equation is of the form:

$$\psi(x) = Ae^{ikx} + Be^{-ikx}, \quad k = \sqrt{\frac{2mE}{\hbar^2}} \qquad (25)$$

This function is not normalizable, since it does not decay for $|x| \rightarrow \infty$. Two properties follow from the impossibility of normalizing this function: (1) The energies are not quantized, i.e. all values $E>0$ are allowed. (2) The energies are degenerate (+k and -k).

2.2   Potential Step

Our next task is to solve the TISE for one-dimensional single-particle system whose potential energy is piecewise constant [11]. A piecewise constant potential is one that is constant for all values of x except at a finite number of discontinuities-points, where it changes from one constant value to another. One of the simplest piecewise-constant potentials is the potential step

$$V(x) = \begin{cases} 0, & x < 0 \\ V_0, & x \geq 0 \end{cases} \rightarrow V(x) = V_0 \Theta(x) \qquad (26)$$
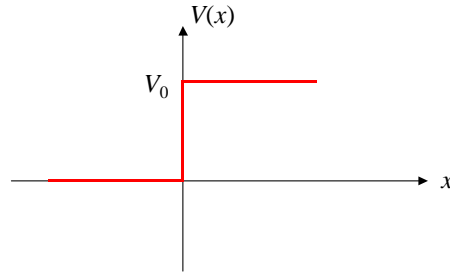
shown graphically in Figure 1-18.

Figure 3. Potential step (an example of a piecewise constant potential).

Our task is to solve the following problem: We assume that we have a beam of particles incident from the left that encounters an impulsive force at $x=0$. We will consider two cases: Case (a) when the energy E of the particle is less than V_0, and Case (b) when the energy of the particle is greater than V_0.

Case (a): $E<V_0$

For this particular case, we need to distinguish between two separate regions:

- On the left from the potential step, $E > V(x)$ ➔ classically-allowed region

- On the right from the potential step, $E < V(x)$ ➔ classically-forbidden region

- $x=0$ is called a turning point ➔ point that separates the classically-allowed from the classically forbidden regions (see the figure below).
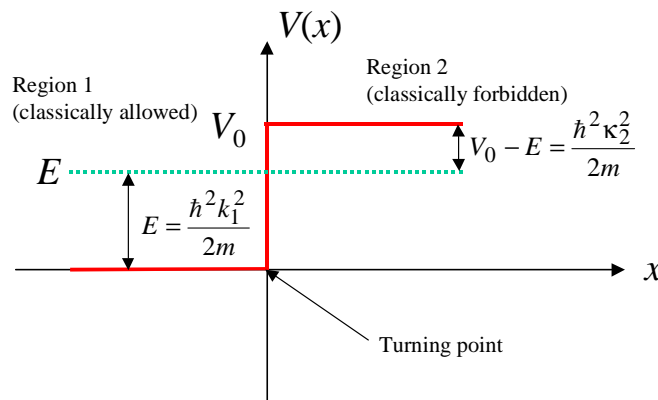

Figure 4 Description of the various regions for case (a).

The solution procedure for this type of problems is the following one:

- Write down the TISE for each region in which the potential energy is constant. Solve the TISE up to arbitrary constants.
- If necessary, apply the asymptotic condition to get physically admissible state function.
- Match the wavefunctions and the derivatives of the wavefunctions at each of the turning points.

Following the above-outlined procedure, we get the following general expressions for the wavefunctions in region 1 ($x < 0$) and region 2 ($x > 0$):

$$\psi(x) = \begin{cases} A^{(1)} e^{ik_1 x} + B^{(1)} e^{-ik_1 x} = \psi_1(x), & k_1 = \sqrt{\dfrac{2mE}{\hbar^2}} \\[4mm] A^{(2)} e^{-\kappa_2 x} = \psi_2(x), & \kappa_2 = \sqrt{\dfrac{2m(V_0 - E)}{\hbar^2}} \end{cases} \tag{27}$$

The unknown coefficients that appear in the above expression are calculated from the requirement that $\psi(x)$ be continuous and smooth, which implies that it must also have continuous first derivative. Therefore, using the boundary conditions:

$$\begin{cases} \psi_1(0) = \psi_2(0) \\[2mm] \dfrac{d\psi_1(x)}{dx}\bigg|_{x=0} = \dfrac{d\psi_2(x)}{dx}\bigg|_{x=0} \end{cases} \tag{28}$$

we get:

$$\begin{cases} B^{(1)} = \dfrac{k_1 - i\kappa_2}{k_1 + i\kappa_2} A^{(1)} \\[3mm] A^{(2)} = \dfrac{2k_1}{k_1 + i\kappa_2} A^{(1)} \end{cases} \tag{29}$$

Some important conclusions that can be derived from the above equations are:

- $\left| B^{(1)} \right| = \left| A^{(1)} \right|$, which means that in region 1, two waves of equal amplitude travel in the opposite direction and with the same phase velocity. Because of this, the wavefunction in region 1 represents a standing wave.

- The above observation suggests that the probability of reflection $R(E)=1$ and that of transmission $T(E)=0$. This result is just what we would expect were we applying classical physics to the problem.

- In region 2, the wavefunction represents an evanescent wave, whose amplitude equals to

$$\left|\psi_2(x)\right| = \frac{2k_1}{\sqrt{k_1^2 + \kappa_2^2}}\left|A^{(1)}\right|e^{-\kappa_2 x} \tag{30}$$

This is consistent with the previous observation that all incident particles with **E<V₀** are reflected back. Therefore, we might say that no probability flow is associated with evanescent waves**.**
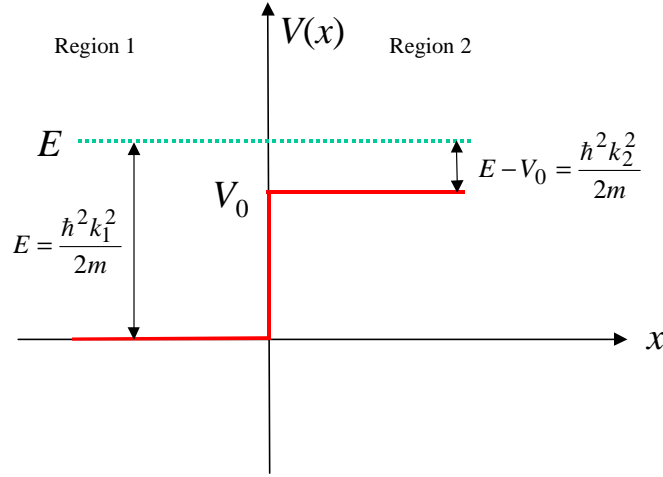
Case (b): $E>V_0$

Figure 5. Graphical description of the variables used for this case.

Following the procedure described above, we get the following general expressions for the wavefunctions in region 1 and region 2:

$$\psi(x) = \begin{cases} A^{(1)}e^{ik_1 x} + B^{(1)}e^{-ik_1 x} = \psi_1(x), & k_1 = \sqrt{\dfrac{2mE}{\hbar^2}} \\ A^{(2)}e^{ik_2 x} = \psi_2(x), & k_2 = \sqrt{\dfrac{2m(E-V_0)}{\hbar^2}} \end{cases} \tag{31}$$

The unknown coefficients that appear in the above expression are again calculated from the requirement that $\psi(x)$ be continuous and smooth, which implies that it must also have continuous first derivative. Therefore, using the boundary conditions:

$$\begin{cases} \psi_1(0) = \psi_2(0) \\ \dfrac{d\psi_1(x)}{dx}\bigg|_{x=0} = \dfrac{d\psi_2(x)}{dx}\bigg|_{x=0} \end{cases} \tag{32}$$

in this particular case we obtain:

$$\begin{cases} B^{(1)} = \dfrac{k_1 - k_2}{k_1 + k_2} A^{(1)} \\ A^{(2)} = \dfrac{2k_1}{k_1 + k_2} A^{(1)} \end{cases} \tag{33}$$

Some important conclusions that can be derived from the above equation are:

- Since all coefficients are real and their magnitude is in general not equal to one, we might conclude that the wavefunction for continuum stationary states is of the following general form:

$$\psi(x) = \begin{cases} \textbf{incident wave} + \textbf{reflected wave} & \rightarrow \textbf{source} \\ \textbf{transmitted wave} & \rightarrow \textbf{detector} \end{cases}$$

We want to define the following two quantities:

- $\rho(E) = B^{(1)} / A^{(1)}$ ➔ reflection probability amplitude

- $\tau(E) = A^{(2)} / A^{(1)}$ ➔ transmission probability amplitude

Then, we can write:

$$\psi(x) = \begin{cases} A^{(1)} e^{ik_1 x} + \rho(E) A^{(1)} e^{-ik_1 x} = \psi_1(x), & x < 0 \\ \tau(E) A^{(1)} e^{ik_2 x} = \psi_2(x), & x \geq 0 \end{cases} \tag{34}$$

From the probability amplitudes, one can calculate the reflection and transmission coefficients. To do so, we return to the probability current densities - the fluxes - for the incident, reflected and transmitted waves. If we use the expression for the probability current, of the form

$$J(x) = -\frac{ie\hbar}{2m} \left(\frac{\partial \psi^*}{\partial x} \psi - \psi^* \frac{\partial \psi}{\partial x} \right) \tag{35}$$

we arrive at the following results:

$$J_1 = -\frac{e\hbar k_1}{2m} \left[1 - |\rho(E)|^2 \right] \left| A^{(1)} \right|^2 = J_{inc} + J_{ref}, \ x < 0 \tag{36}$$

$$J_2 = -\frac{e\hbar k_2}{2m} |\tau(E)|^2 \left| A^{(1)} \right|^2 = J_{trans}, \ x \geq 0 \tag{37}$$

If we look at the result at region 1, the probability current density J_1 equals the sum of the incident current and a reflected current. In region 2, we have a transmitted current J_2. We can, therefore, define a reflection probability $R(E)$ and transmission probability $T(E)$ in the following manner:

$$R(E) = \left| \frac{J_{ref}}{J_{inc}} \right| = \left| \frac{-\dfrac{q\hbar k_1}{m} |\rho(E)|^2 |A^{(1)}|^2}{-\dfrac{q\hbar k_1}{m} |A^{(1)}|^2} \right| = |\rho(E)|^2 \text{, and} \tag{38}$$

$$T(E) = \left| \frac{J_{trans}}{J_{inc}} \right| = \left| \frac{-\dfrac{q\hbar k_2}{m} |\tau(E)|^2 |A^{(1)}|^2}{-\dfrac{q\hbar k_1}{m} |A^{(1)}|^2} \right| = \frac{k_2}{k_1} |\tau(E)|^2 \ . \tag{39}$$

Since a particle is either reflected or transmitted, we must have that

$$T(E)+R(E)=1 \ . \tag{40}$$

For our particular problem, this gives us:

$$R(E) = \left(\frac{k_1 - k_2}{k_1 + k_2} \right)^2 \text{ and } T(E) = \frac{4 k_1 k_2}{(k_1 + k_2)^2} \ . \tag{41}$$

Therefore, in contrast to the case $E<V_0$, our result for $E>V_0$ does not conform to the predictions of classical physics.
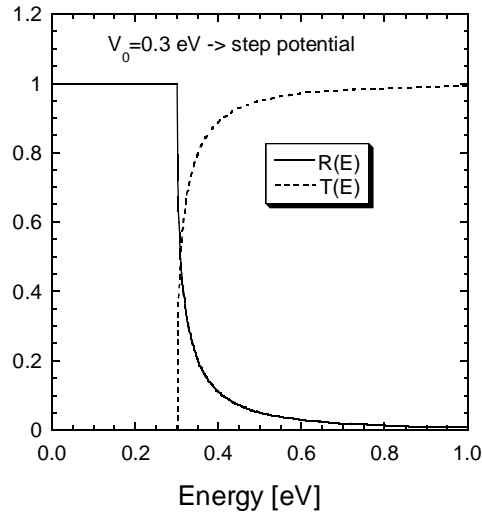

Figure 6 A step potential of height V_0=0.3 eV. The effective mass of the electrons is assumed to be 0.067 m_0, where m_0 is the free electron mass. Transmission and reflection coefficient for a step potential as a function of the incident carrier energy.

An interesting thing to plot is the magnitude squared of the wavefunctions in regions (1) and (2) as a function of position. The behavior of $|\psi_i(x)|^2$ (i=1 for region 1 and i=2 for region 2) is shown on Figure

1-22. We use E=0.25 eV and $A^{(1)}$=1. Note that the energy of the particles E is smaller than the barrier height. Therefore, we expect to see standing wave pattern in region 1 [since $R(E)$=1 for this case] and evanescent (exponentially-decaying solution) in region 2.
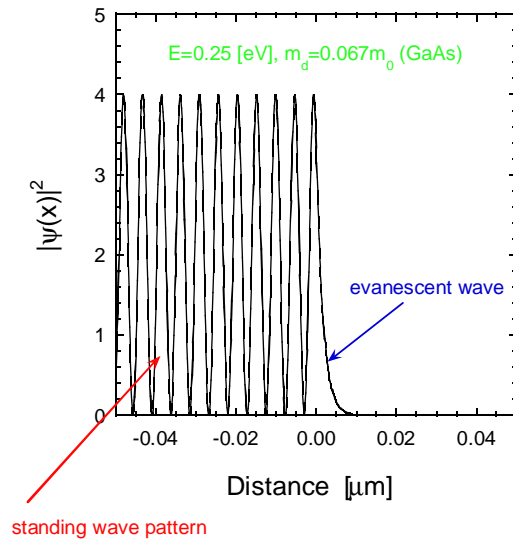

Figure 7. The magnitude squared of the wavefunction for carrier energy less than the barrier height.

2.3   *Tunneling Through a Single Barrier*

Consider the potential barrier shown in Figure1-23, for which the potential energy term appearing in the 1D TISE is of the form:

$$V(x) = \begin{cases} 0, & x < 0 \\ V_0, & 0 \le x \le L \\ 0, & x > L \end{cases}$$

(42)

Following the steps outlined in the previous section, it is easy to show that for energies $E<V_0$, the general solution of the 1D TISE in each of the three regions, is of the form:

$$\psi_1(x) = Ae^{ikx} + Be^{-ikx}$$
$$\psi_2(x) = Ce^{-\gamma x} + De^{\gamma x}, \quad \text{where } k = \sqrt{\frac{2mE}{\hbar^2}} \quad \text{and} \quad \gamma = \sqrt{\frac{2m(V_0 - E)}{\hbar^2}}. \qquad (43)$$
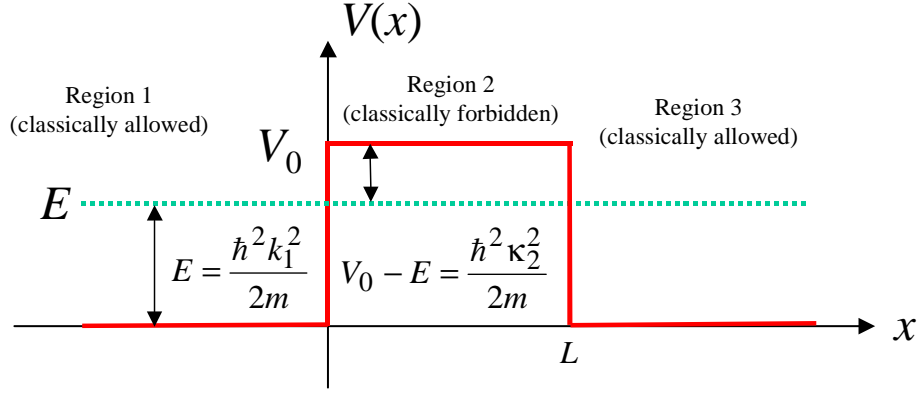$$\psi_3(x) = Ee^{ikx} + Fe^{-ikx}$$

Figure 8. Single potential barrier.

The application of the continuity conditions of the wavefunction at the boundaries $x = 0$ and $x = L$, leads to the following relationship between the unknown constants:

$$
\begin{aligned}
\psi_1(0) = \psi_2(0) \quad &\rightarrow \quad A + B = C + D \\
\psi_1'(0) = \psi_2'(0) \quad &\rightarrow ik(A - B) = -\gamma(C - D) \\
\psi_2(L) = \psi_3(L) \quad &\rightarrow \quad Ce^{-\gamma L} + De^{\gamma L} = Ee^{ikL} + Fe^{-ikL} \\
\psi_2'(L) = \psi_3'(L) \quad &\rightarrow \quad -\gamma\left(Ce^{-\gamma L} - De^{\gamma L}\right) = ik\left(Ee^{ikL} - Fe^{-ikL}\right)
\end{aligned}
\qquad (44)
$$

Using the above four equations, we can find the relationships between various coefficients, i.e. using matrix representation these relationships can be represented as:

$$
\begin{bmatrix} A \\ B \end{bmatrix} =
\begin{bmatrix}
\frac{1}{2}\left(1 + i\frac{\gamma}{k}\right) & \frac{1}{2}\left(1 - i\frac{\gamma}{k}\right) \\
\frac{1}{2}\left(1 - i\frac{\gamma}{k}\right) & \frac{1}{2}\left(1 + i\frac{\gamma}{k}\right)
\end{bmatrix}
\begin{bmatrix} C \\ D \end{bmatrix} = M_1 \begin{bmatrix} C \\ D \end{bmatrix}
$$

$$
\begin{bmatrix} C \\ D \end{bmatrix} =
\begin{bmatrix}
\frac{1}{2}\left(1 - i\frac{k}{\gamma}\right)e^{(ik+\gamma)L} & \frac{1}{2}\left(1 + i\frac{k}{\gamma}\right)e^{-(ik-\gamma)L} \\
\frac{1}{2}\left(1 + i\frac{k}{\gamma}\right)e^{(ik-\gamma)L} & \frac{1}{2}\left(1 - i\frac{k}{\gamma}\right)e^{-(ik+\gamma)L}
\end{bmatrix}
\begin{bmatrix} E \\ F \end{bmatrix} = M_2 \begin{bmatrix} E \\ F \end{bmatrix}
$$
$$(45)$$

In other words, we have the following relationship between the coefficients *A* and *B*, and the coefficients *E* and *F*:

$$\begin{bmatrix} A \\ B \end{bmatrix} = M_1 \begin{bmatrix} C \\ D \end{bmatrix} = M_1 M_2 \begin{bmatrix} E \\ F \end{bmatrix} = M \begin{bmatrix} E \\ F \end{bmatrix}, \tag{46}$$

where the matrix M has elements m_{ij}. Therefore, for coefficients A and E (using the asymptotic condition that $F=0$) we have the following simple relationship: $A=m_{11}E$, i.e. the transmission coefficient is simply given by:

$$T(E) = \left| \frac{E}{A} \right|^2 = \frac{1}{|m_{11}|^2}. \tag{47}$$

After a rather straightforward calculation, we arrive at the following expression for the transmission coefficient for particle energies less than the barrier height:

$$T(E) = \left[1 + \left(\frac{\gamma^2 + k^2}{2k\gamma} \right)^2 sh^2(\gamma L) \right]^{-1} \tag{48}$$

In the case of a weak barrier ($\gamma L \ll 1$), the expression for the transmission coefficient simplifies to:

$$T(E) \approx \frac{1}{1 + (kL/2)^2}. \tag{49}$$

In the opposite limit, i.e. when the barrier is very strong (γL is very large), we have the following approximate expression for the transmission coefficient:

$$T(E) \approx \left(\frac{4k\gamma}{k^2 + \gamma^2} \right)^2 \exp(-2\gamma L). \tag{50}$$

For energies larger than the barrier height, i.e. $E > V_0$, using that $\gamma = ik_2$, gives:

$$T(E) = \left[1 + \left(\frac{k^2 - k_2^2}{2kk_2} \right)^2 \sin^2(k_2 L) \right]^{-1}. \tag{51}$$

The later result is similar to the one obtained in the previous section, i.e. the transmission maxima ($T(E)=1$) occur for $k_2 L = n\pi$.

In Figure 1-24, top panel, we show several results for a potential barrier. The barrier height equals V_0=0.4 eV, whereas the barrier width is L=6 nm. We also show how the transmission coefficient varies with the width of the barrier, for fixed E and V_0 (Figure 1-24, bottom panel). We consider two cases: particle energies smaller and larger than the barrier height.
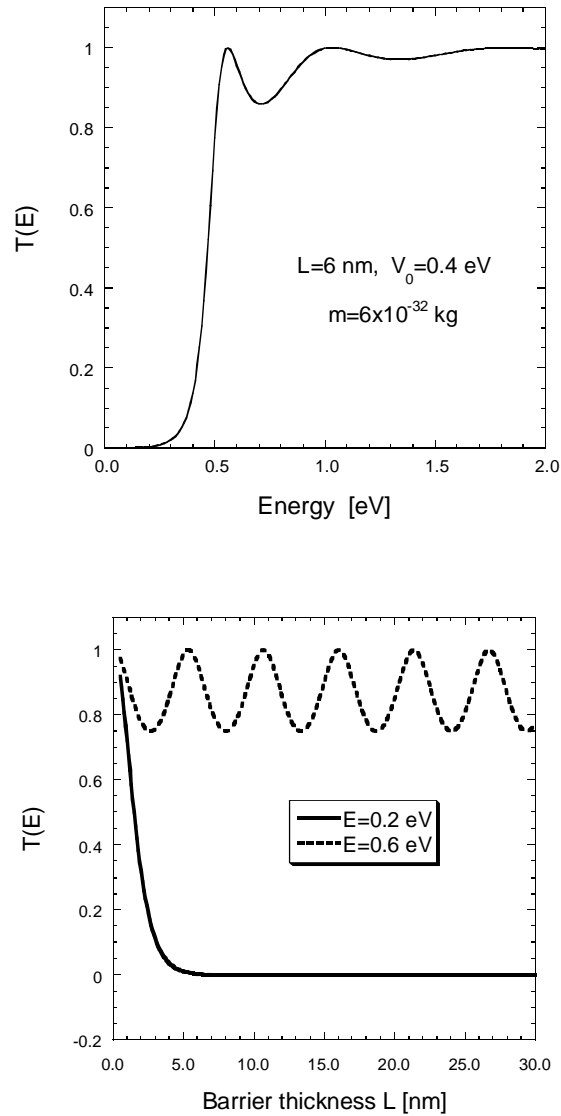

Figure 9. Top panel - Variation of the transmission coefficient with energy. Bottom panel - Variation of the transmission coefficient with the barrier thickness.

The following observations can be derived from the results presented in this section:

- Classical physics would predict that no particles with energy $E<V_0$ are transmitted; quantum physics reveals that the probability of transmission of such particles increases hyperbolically with increasing energy.

- Classical physics would predict that all incident particles with $E>V_0$ are transmitted; quantum mechanics shows that this condition - called **total transmission** - occurs only at a few discrete energies. An incident particle with $E>V_0$ that lies between these special values, determined by the condition $k_2 L = n\pi$, may be reflected. The probability of reflection decreases very rapidly with increasing the energy of the particle E.

- For another perspective on transmission and reflection by a barrier, now let us look at the results shown in Figure 1-24, bottom panel. Here, the energy of the particle E and the barrier height are fixed and $T(E)$ is plotted as a function of the barrier width L. This figure shows another bizzare result: for a given energy E, only barriers of certain width will transmit all particles of this energy (transparent barriers). But there is no value of the width such that a barrier of this width reflects all incident particles, because for all values of L, the reflection coefficient $R(E)$ is less than one.

- Because of the hyperbolic decay of the eigenfunction in the classically forbidden region, the amplitude of the eigenfunction in the detector region is reduced from its value in the source region.

2.4   *Tunneling Through Arbitrary Piecewise-Constant Barrier*

We now consider the case of arbitrary number of piece-wise constant potential barriers. As in the case of a simple barrier, the transmission and the reflection coefficients are calculated by solving, either explicitly or implicitly the Schrödinger equation over the domain $x_L < x < x_R$. We assume that outside of the domain of interest (in the asymptotic regions), the wavefunction consists of superposition of traveling waves, and we write the general solution

$$\psi(x) = \begin{cases} a_l e^{ik_l(x-x_l)} + b_l e^{-ik_l(x-x_l)}, & x < x_l \\ a_r e^{-ik_r(x-x_r)} + b_r e^{ik_r(x-x_{rl})}, & x > x_r \end{cases} \tag{52}$$

In the transmission matrix approach outlined in the previous section, the domain is divided into a suitable number of intervals over each of which the potential can be taken to be constant, or perhaps linearly varying. Within each such interval, the wavefunction is expanded in terms of two independent solutions at the chosen energy (oppositely directed traveling waves if the potential is constant). Then the amplitudes of these waves at the two ends of interval i can be related by the propagation matrix P_i:

$$P_i = \begin{bmatrix} e^{ik_i l_i} & 0 \\ 0 & e^{-ik_i l_i} \end{bmatrix} \tag{53}$$

The appropriate matching conditions at the boundary between intervals i and $i+1$ must be derived from the form of the Hamiltonian, and are expressed by a matrix B_i which is typically of the form

$$B_i = \frac{1}{2}\begin{bmatrix} 1+r & 1-r \\ 1-r & 1+r \end{bmatrix} \tag{54}$$

where $r = v_i / v_{i+1}$, is the velocity ratio. One can then relate the coefficients in the left asymptotic region, incorporate into a vector $\psi_l = [a_l, b_l]^T$, to those in the right asymptotic region, $\psi_r = [b_r, a_r]^T$, by a matrix M formed from the product of the appropriate propagation and boundary matrices:

$$\Psi_r = M\Psi_l = P_m B_{m-1} \dots B_2 P_2 B_1 P_1 \Psi_r \tag{55}$$

In practical calculations, the transmission matrix approach has proven to be less than satisfactory, because it is prone to arithmetic overflow. In regions where the wavefunction is evanescent, the P matrices contain real elements equal to the attenuation of the region and its inverse. The inverse is likely to be a very large positive number, and if several evanescent regions are cascaded, the numbers in the matrix will rapidly exceed the dynamic range of floating point variables. This problem is particularly severe when the transmission matrix scheme is applied to multi-band models, because at any given energy many of the bands will be evanescent, but it has also been observed in simple single-band calculations. The transfer matrix method [12,13] has been generalized to multi-dimensional systems by Frensley [1,14], Lent et al. [15], and to multi-band Hamiltonians by Ting et al. [16,17]. In the latter methods the scattering boundary conditions are applied via the quantum transmitting boundary method (QTBM) [18], and the transmission is obtained via the solution of a linear system with dimensions proportional to the size of the device that has to be solved repeatedly. Very recently, a modified version of the QTBM has been developed that expands the scattering solutions in terms of two different closed system wave functions [19]. The calculations are charge self-consistent, but have only been implemented for single-band situations so far.

The second class of simulators is based on the Green's function method to calculate the quantum transport properties, with the coupling to the leads being introduced via the self-energy. The advantage of this approach is the well developed theory of the Green's functions that also allows one to consider inelastic scattering within the nonequilibrium Green's function formalism. A very efficient and widely used algorithm is the recursive Green's function method [20] that has been successfully implemented for two-dimensional devices [21,22] and for small three-dimensional structures such as nano-wires [23]. It's main advantage is that it does not only yield the retarded Green's function that is connected to the S- or T-matrix, but also the less-than Green's function [21], which is needed if inelastic scattering to be

considered. The main drawback of the method is its restriction to devices that can be discretized into cross-sectional slices with nearest neighbor interactions only, a condition that cannot be maintained for structures with more than two contacts, since additional contacts inevitably couple more distant slices with one another. For a detailed review of this method please see the article by Lake *et al*. [20]. Thus, although a large variety of methods has been developed in the past decades, the quantum-mechanical ballistic multi-band transport calculation of large two- and three-dimensional structures or devices with more than two Ohmic contacts still presents a significant challenge.

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